



# Polarized neutrons and high magnetic fields on TAS IN22

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**PINS Workshop**

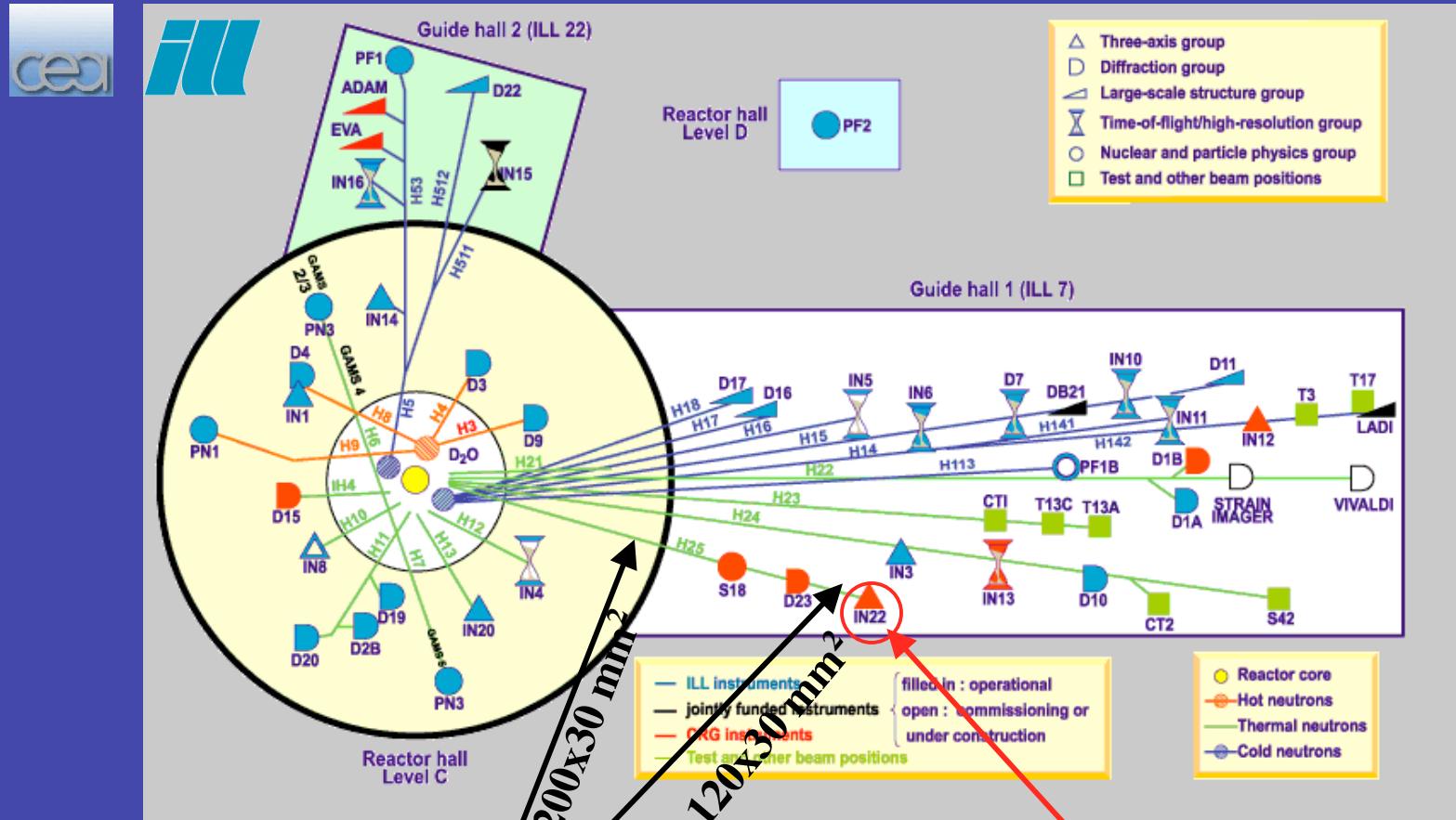
**BNL**

**6-7 April 2006**

# OUTLINE

- Polarized neutron configuration on IN22
  - Heusler-based polarization and polarization analysis
- Exemples in LPA (Heusler/Helmholtz configuration)
  - Magnetic and lattice excitation spectra in YBCO near optimal doping
  - Magnetic and lattice excitations in the ladders of  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$
- High-field and SNP configurations
- Conclusion

# IN22 (ILL7 guide hall)

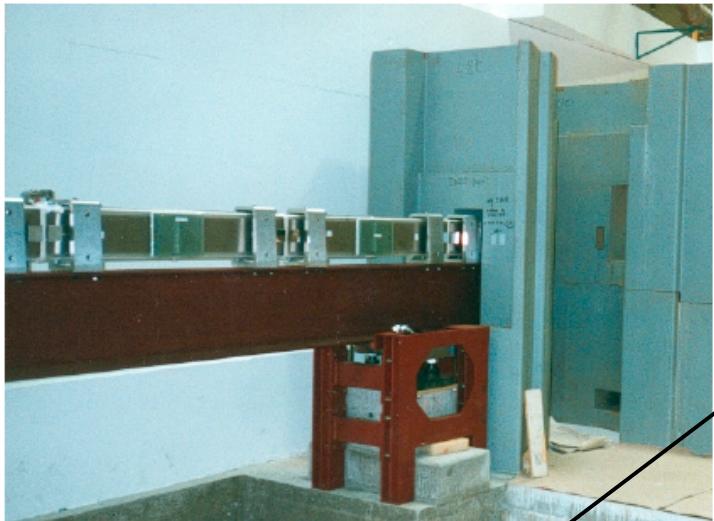


H25 supermirror (SM) guide  
(thermal neutrons)

TAS IN22  
Polarized three-axis

# H25 m=2 supermirror (SM) guide (1995&2006)

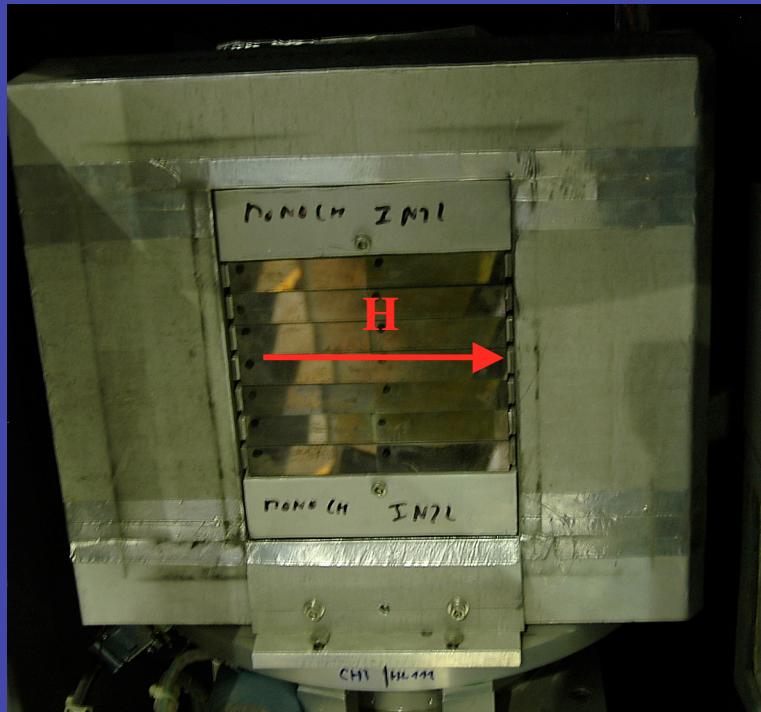
H25 GUIDE: PART BETWEEN D23 AND IN22



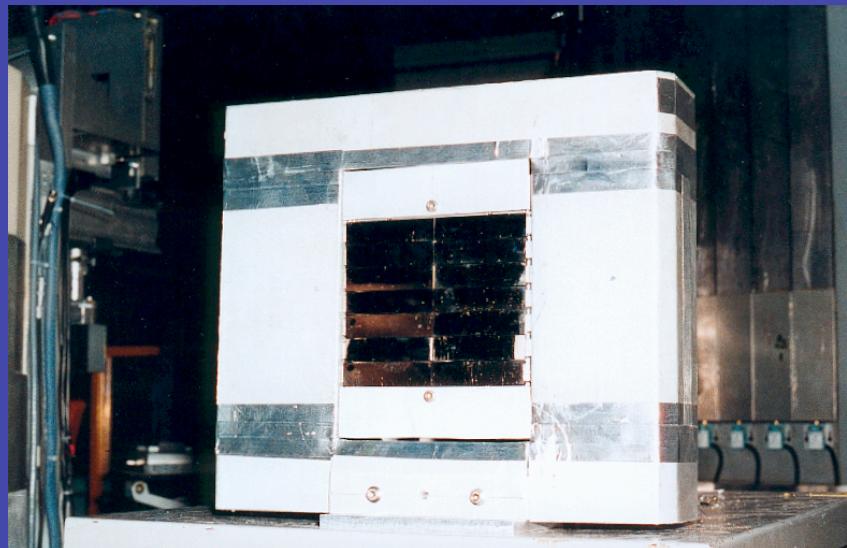
- Length: 65 m
- Section: 20x3 (60 m; carter)  
12x3 (5m)
- Curvature radius: 9 km
- SM Ni-Ti (m=2):  
CILAS (60 m; 1995)  
& SWISS-NEUTRONICS (5 m; 2006)
- Flux @ mono:  $2.5 \times 10^9$  n/cm<sup>2</sup>/s
- Divergence:  $\sim 0.2 \lambda_i (\text{°}, \text{\AA})$  (0.2°@ 1 Å)

3 monoch: { PG002  
                  Cu111  
                  HL111 }

# Polarized neutrons on IN22



Monochromator/polarizer:  
Heusler-based



- Horizontal field.  $H \approx 1.7$  kG at gap center
- $L(\text{mm}) \times H(\text{mm}) = 150 \times 120$
- Vertical focusing (variable; 7 blades); Flat horizontal
- Heusler crystals: 14 pieces  $7.5 \times 1.7 \times 0.5 \text{ cm}^3$ ;  $\eta_h: \approx 0.3\text{-}0.4^\circ$   
 $\eta_v: \approx 0.5\text{-}0.7^\circ$
- Polarization:  $P \approx 0.94\text{-}0.96$  depending on  $k_i$

# Flux at sample position

(x 10<sup>7</sup> n/cm<sup>2</sup>/s)

$k_i$ (Å <sup>-1</sup> )	1.5	1.64	1.97	2.662	4.1	6.0
<b>Monoch</b>						
<b>PG002</b>	0.6	0.8	1.7	3.5	6.0	2.5
<b>HL111</b>	0.15	0.2	0.4	0.7	1.2	0.4
<b>Cu111</b>	-	-	0.6	1.2	2.0	1.0

Monoch-Sample distance ≈ 1.8 m

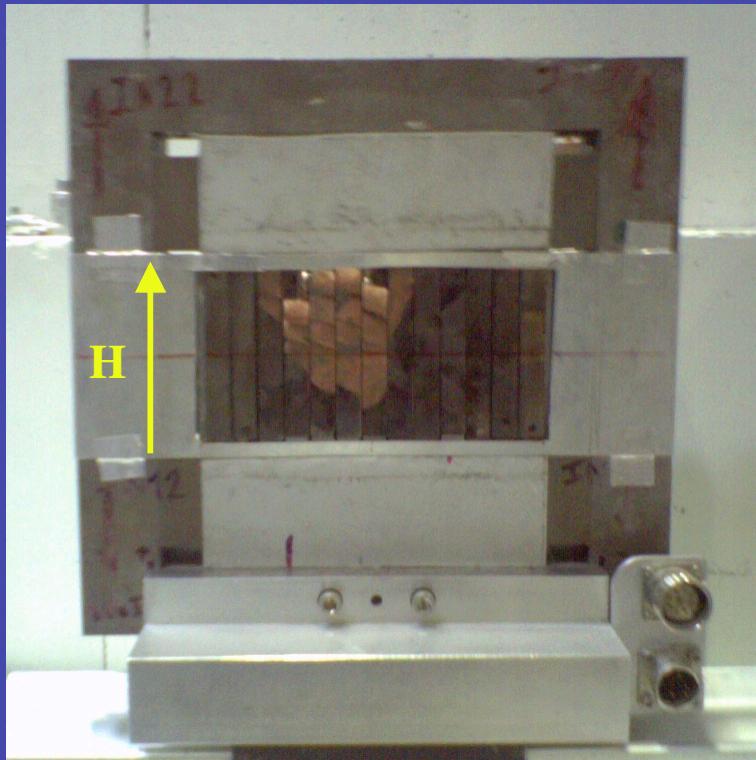
**PG002/HL111 ≈ (2 to 3)x2**

**PG002/Cu111 ≈ 3**

**Flux maximum at  $k_i \approx 4.1 - 4.5$  Å<sup>-1</sup>**

## IN22/IN12 "old" Heusler analyser

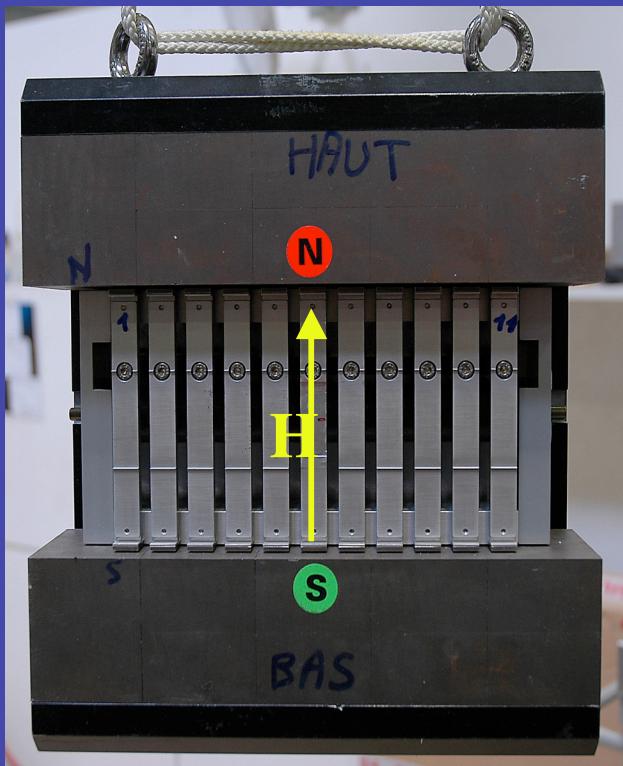
(1998)



- Optimized for "coldish" neutrons (usable on IN22 and IN12)
- Overall dimensions: 270x260 mm<sup>2</sup>
- Vertical field  $\approx 2.1$  kG
- Dimensions: 150x80 mm<sup>2</sup>:
  - 13 blades 11x80x5 mm<sup>3</sup> each
  - Heusler mosaic:  $\eta_h: \approx 0.3^\circ$
- Focusing:
  - Variable horizontal
  - Flat vertical

# IN22 new analyser: Magnetic circuit and focusing mechanics

(mid 2006)



- Optimized for  $k_f \approx 2.7 \text{ \AA}^{-1}$
- Dimensions: LxH=190x100 mm<sup>2</sup>
- Magnetic field at gap center:  
Vertical,  $B = 3\text{k G}$
- Double focusing:
  - 11 blades: 17x100x5 mm<sup>3</sup> each
  - Variable horizontal focusing
  - Fixed vertical focusing  
(optimized for  $2.662 \text{ \AA}^{-1}$ )
- Heusler mosaic:  $\eta_h \approx 0.5^\circ$

Expected gain in count rates: 2 to 3, depending on  $k_f$

## Tests of new Heusler crystals (IN22 analyser)

( $\mathbf{X}^{\text{tals}}$  produced by P. Courtois/SON\_ILL)

### Configuration:

PG002 Monochromator-----> Sample in -----> HL111 Analyser----> Detector  
3-kG magnet

Beam size: LxH = 30x30 mm<sup>2</sup>

Beam divergence:  $\alpha_2 \approx 0.5^\circ$

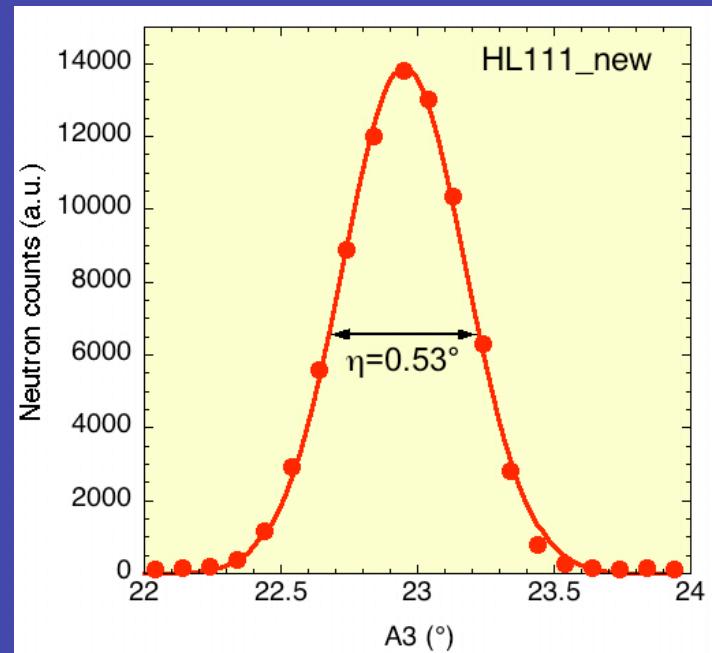
- **HL111 40x17x5 mm<sup>3</sup>:**

Average on ~12 crystals:

Mosaic:  $\eta_H = 0.55^\circ \pm 0.1^\circ$

Polarization:  $P = 0.95 \pm 0.02$

Intensity:  $I_{\max} \approx 8000-10000$  (a.u.)



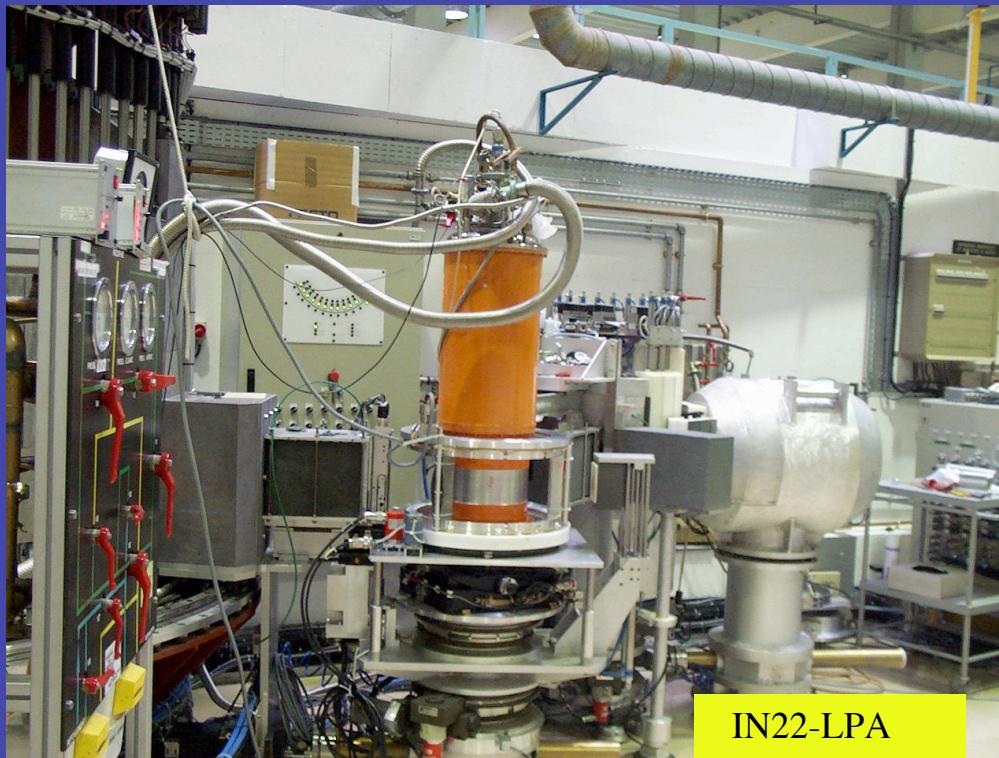
- **PG002 40x17x2 mm<sup>3</sup>:**  $\eta_H \approx 0.50^\circ$  Intensity  $\approx 20000$  (a.u.)

Reduction factor in reflectivity (HL/PG):  $\approx 2-2.5$

→ Slightly improved (~factor of 1.2)

# Longitudinal Polarization Analysis (LPA) Configuration

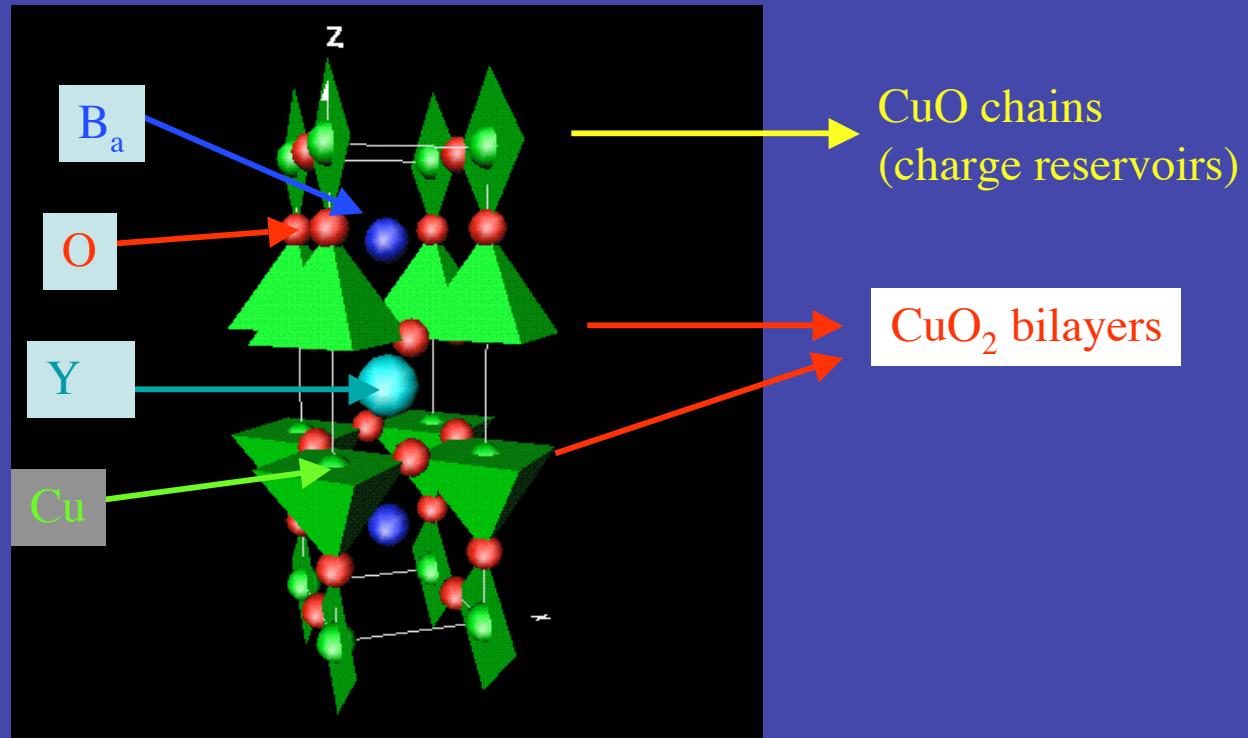
Heusler-Helmholtz-Heusler configuration



- Best flipping ratio on a Bragg peak: 30 at  $2.662 \text{ \AA}^{-1}$
- Best flipping ratio on a magnetic excitation: 25 at  $2.662 \text{ \AA}^{-1}$
- Polarisation analysis doable from  $E_i \approx 5 \text{ meV}$  to  $E_i \approx 90 \text{ meV}$

Exemples: **Yba<sub>2</sub>Cu<sub>3</sub>O<sub>6+x</sub>**, La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub>, CuGeO<sub>3</sub>, **Sr<sub>14</sub>Cu<sub>24</sub>O<sub>41</sub>** ...

# Magnetic/Structural separation in the High- $T_c$ $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

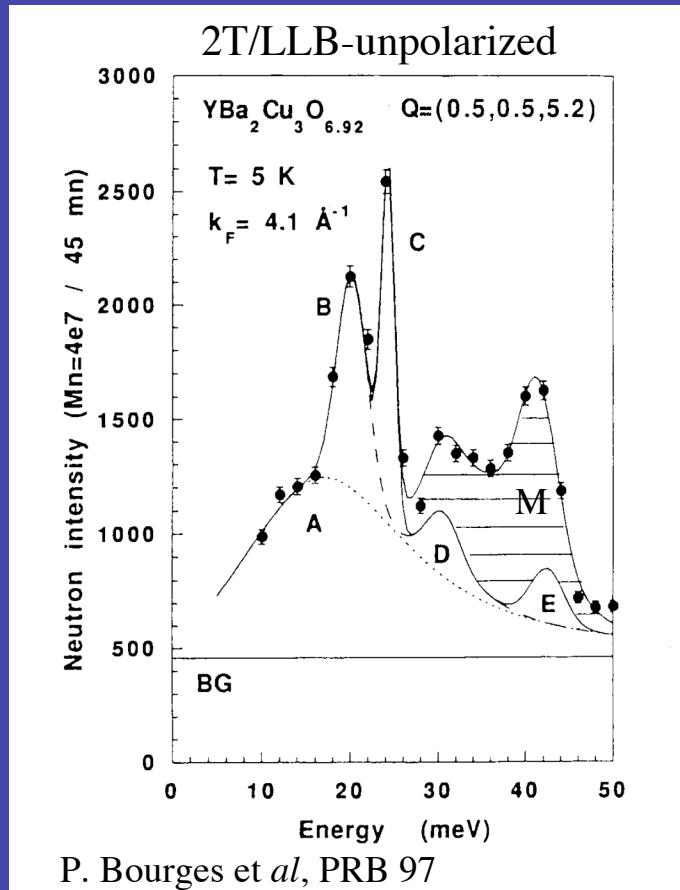


- Insulating for  $x \approx 0$
- High- $T_c$  superconductivity appears for  $x > 0.4$  :  $T_c \approx 93$  K for  $x_{\text{opt}} \approx 0.92$

**Key problem:** does the magnetism plays a role in the pairing mechanism?

**Solution:** Determine separately the **lattice** and **magnetic** excitation spectra

# Magnetic/Structural separation in the high- $T_c$ $\text{YBa}_2\text{Cu}_3\text{O}_{6.92}$

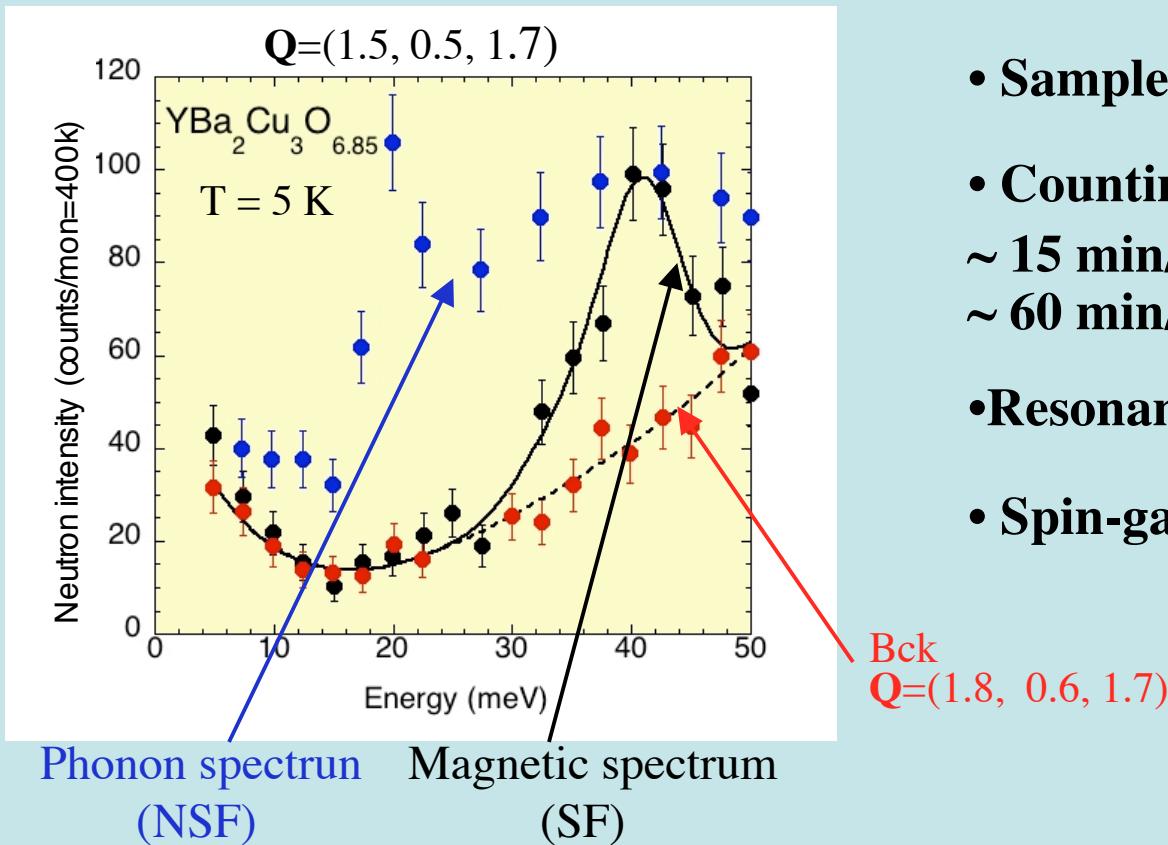


- Superconducting material ( $T_c \approx 92 \text{ K}$ )
- Superposition of several contributions
  - Nuclear Bragg peaks (C)
  - Phonons (B, D, E)
  - Other lattice excitations (A)
  - Magnetic excitations (M)
- Problem: determine precisely and independently the magnetic and lattice excitation spectra

Polarized INS with  $\mathbf{P}_i // \mathbf{Q}$ :  
- Magnetic excitations SF  
- Structural excitations NSF

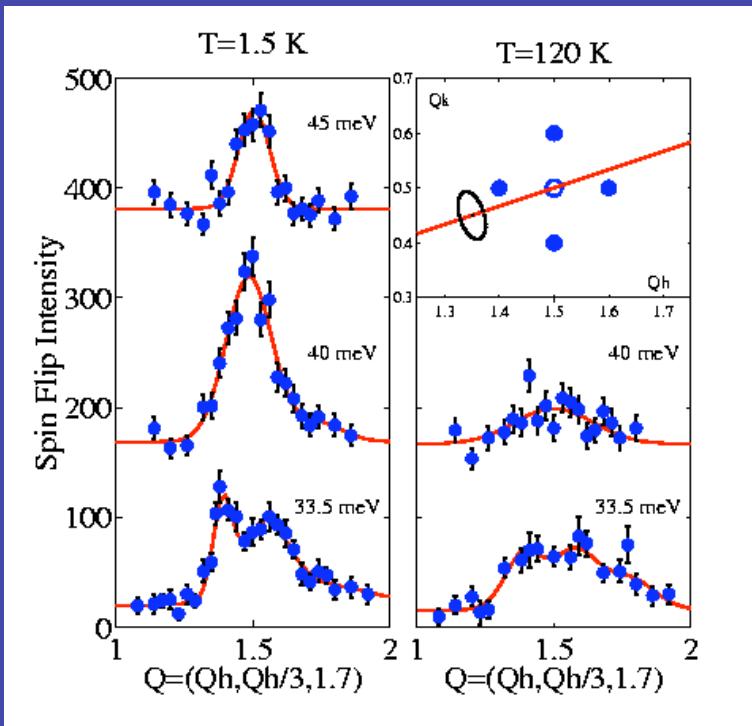
# Separation magnetic/structural in $\text{YBa}_2\text{Cu}_3\text{O}_{6.85}$ ( $T_c \approx 89$ K)

LPA with  $\mathbf{P}_0 \parallel \mathbf{Q}$   $\left\{ \begin{array}{ll} \text{Magnetism} & \text{SF} \\ \text{Lattice} & \text{NSF} \end{array} \right.$



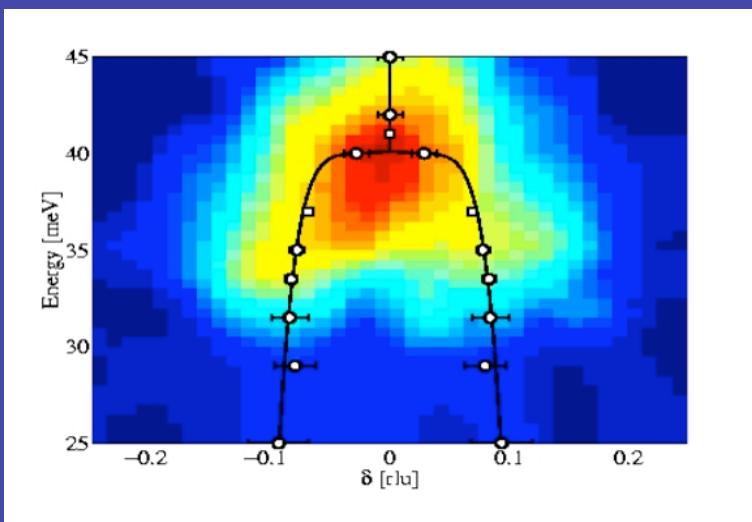
- Sample volume:  $\sim 2$  cc
- Counting times:
  - ~ 15 min/point at 10 meV)
  - ~ 60 min/point at 50 meV
- Resonant mode at  $E_r \approx 41$  meV
- Spin-gap  $E_g \approx 25\text{-}30$  meV

# Spin-flip intensity below and above $T_c$ ( $\approx 89$ K)



LPA with  $P_0 // Q$  : magnetism all SF

- Incommensurate inelastic magnetic correlations between  $E_g$  and  $E_r$
- Resonance peak vanishing at  $T_c$
- IC strongly reduced at  $T_c$  ( $\neq$  LSCO)



Excitation spectrum above  $E_r$ ?

Polarized INS:

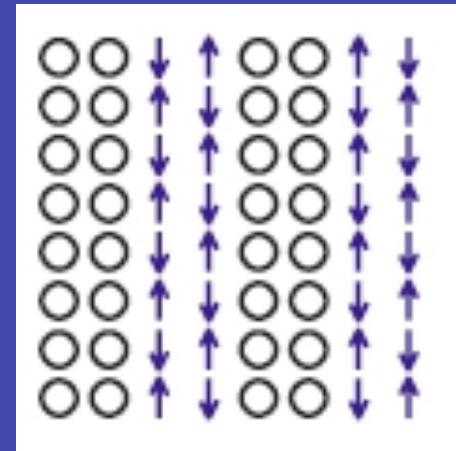
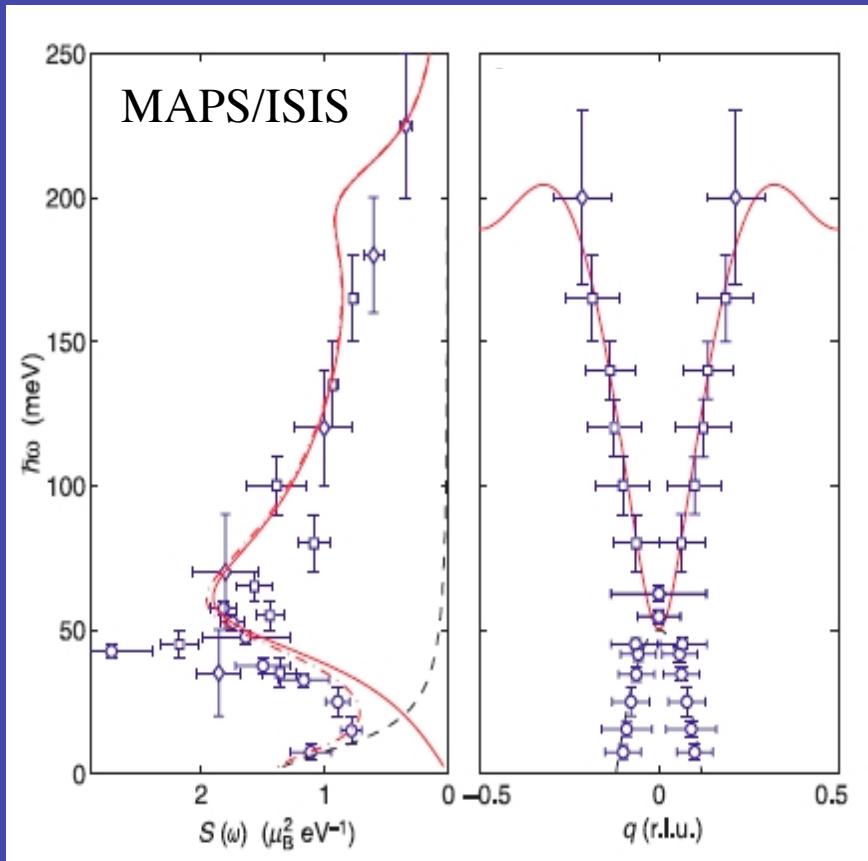
H.M. Rønnow, LPR et al., ILL Annual Report (2000)

Unpolarized INS:

H.A. Mook et al., Nature 395, 580 (1998)

P. Bourges et al., Science 288, 1234 (2000)

## $\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4$ ( $T_c \approx 3\text{-}6 \text{ K}$ )



Stripes and 2-leg spin-ladders

J. Tranquada et al., Nature **429**, 534 (2004)

Similar results:

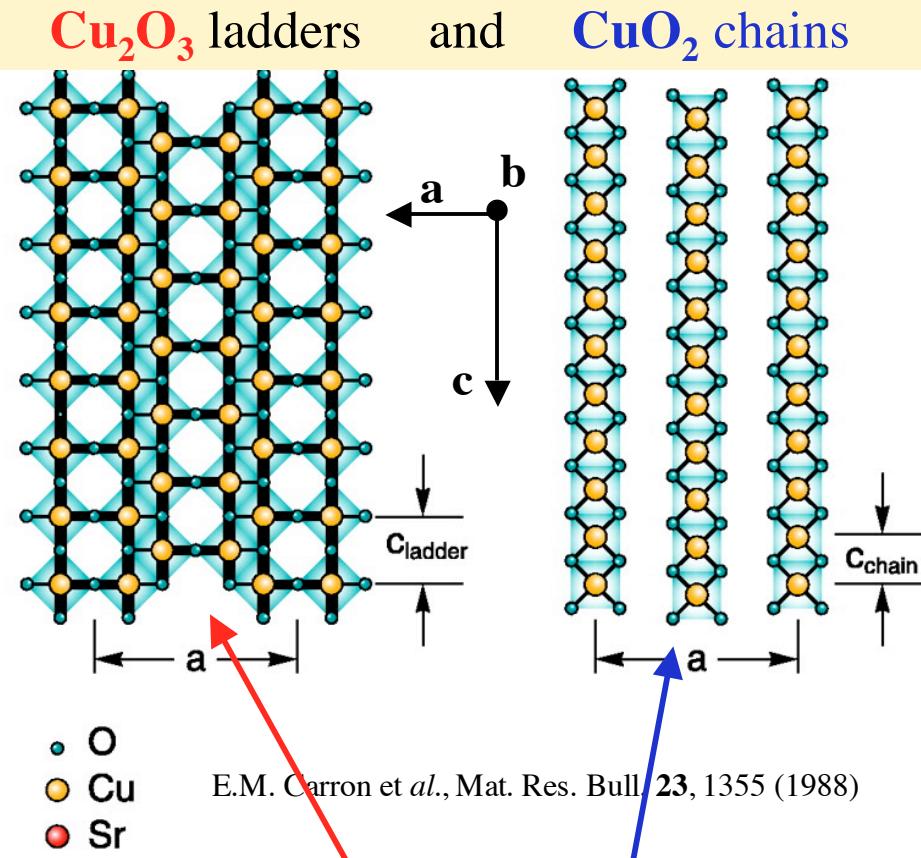
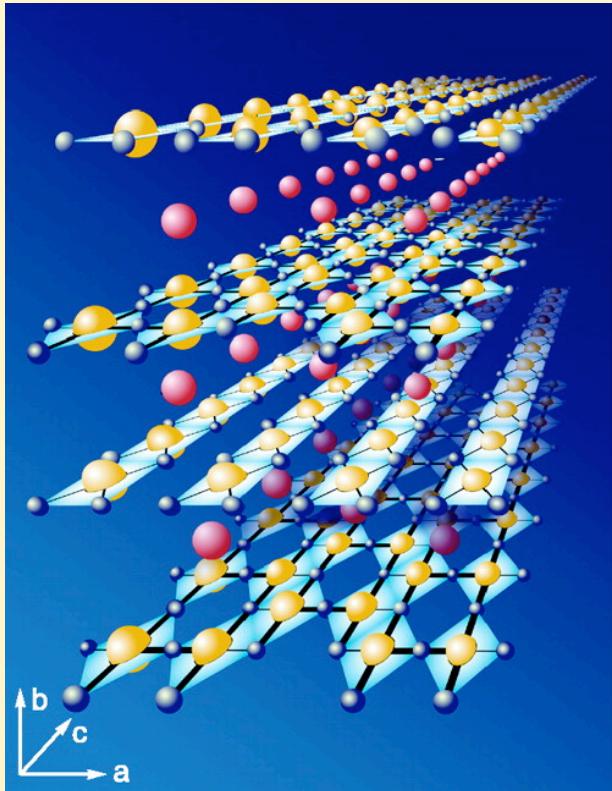
$\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$  ( $T_c \approx 63 \text{ K}$ ;  $E_r \approx 34 \text{ meV}$ )

S. Hayden et al., Nature **429**, 531 (2004)

$\text{La}_{1.84}\text{Sr}_{0.16}\text{CuO}_4$  ( $T_c \approx 38 \text{ K}$ )

N.B. Christensen et al., Phys. Rev. Lett. **93**, 147002 (2004)

# Magnetic/structural excitations in the ladders in $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$



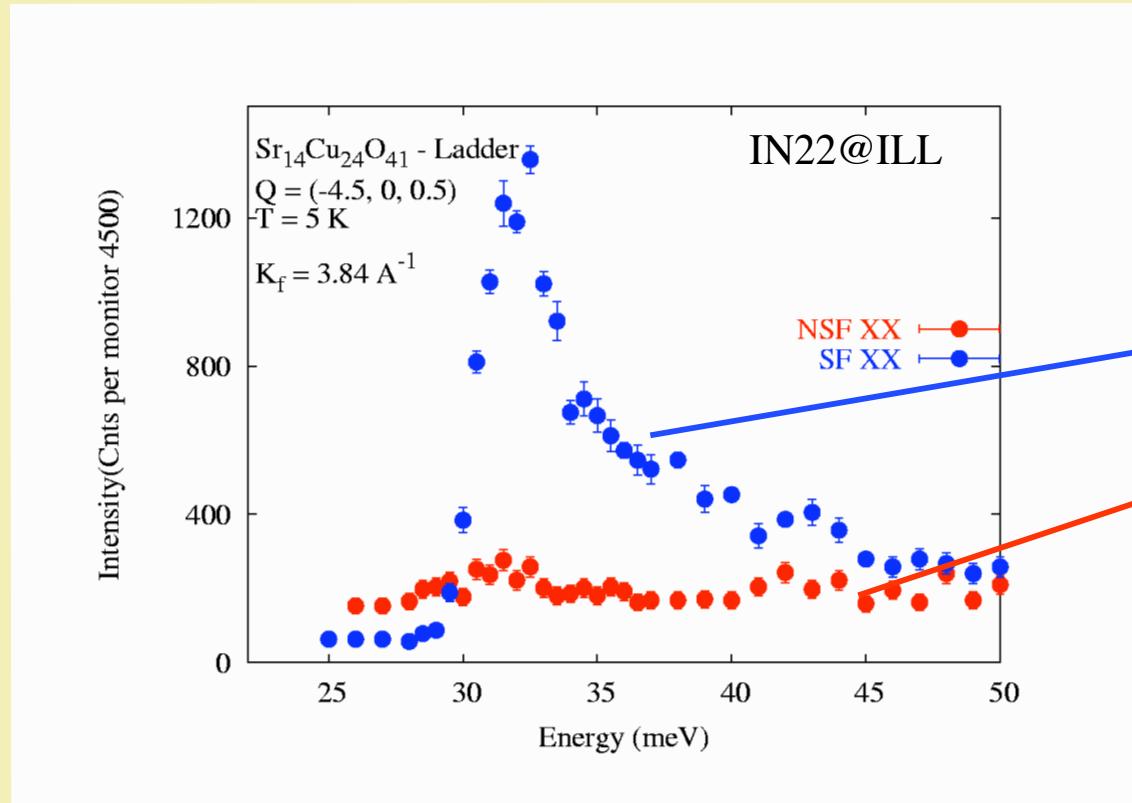
Interest:

- 60% of holes in the  $\text{CuO}$  chains.
- Superconducting under pressure by substitution of Sr for Ca  
( $\text{Sr}_2\text{Ca}_{14}\text{Cu}_{24}\text{O}_{41}$  :  $T_c \approx 6$  K at  $p = 30$  kbar)
- Structure reminiscent of that of  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$



# Separation of structural/magnetic contributions in $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$

- Non-magnetic singlet ground state; singlet-triplet gap:



For  $\mathbf{P}_i$  parallel to  $\mathbf{Q}$  (xx):

- Magnetism SF
- Structural NSF

Magnetic excitations:

Gap at 32 meV

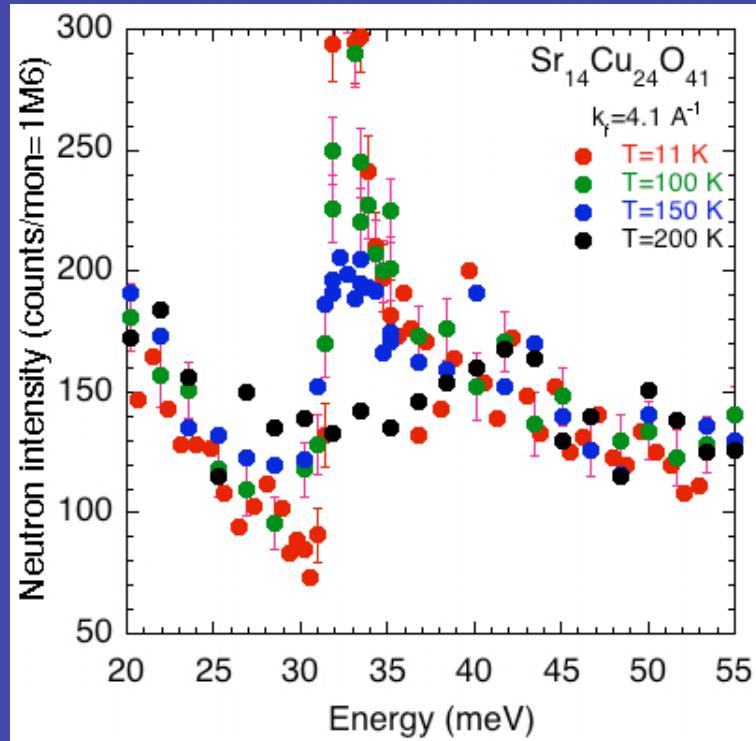
Tail up to 200 meV (dispersion + continuum?)

Lattice excitations:

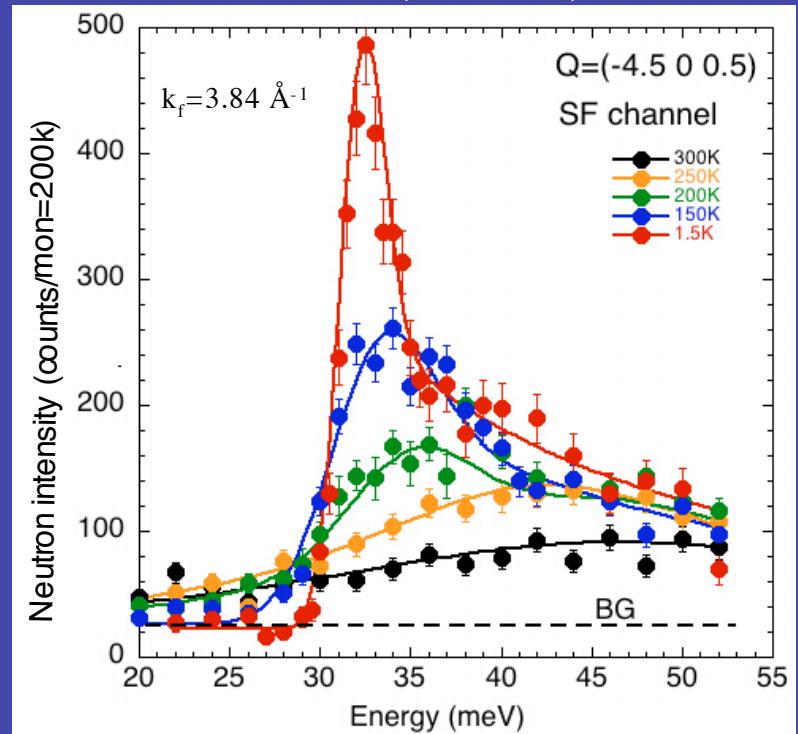
Continuum of LO and TO phonons

# Temperature dependence of ladder excitations

1T/LLB (with Cu111)



IN22/ILL (with HL)



Unpolarized INS:

Phonons+magnetic excitations

Polarized INS ( $\mathbf{P} // \mathbf{Q}$ ):

Only magnetic excitations

- Sharp spin-gap at 1.5 K:  $\Delta \approx 32 \text{ meV}$
- Vanishing between 200-250 K
- Broad feature at high 300 K:  $E_{\max} \sim 50 \text{ meV} \sim 0.5 J_{\text{ladder}}$

# Spherical Polarisation Analysis (SNP) configuration

CRYOPAD on TAS IN22



Polarized neutron optics

- Control  $P_i$  and  $P_f$  independently
- Very compact configuration
- Very low background ( $\sim 20$  n/hour on  $\text{CuGeO}_3$ )
- Very high accuracy on the L-components ( $P_{xx}$ ,  $P_{yy}$  and  $P_{zz}$  at  $\pm 0.002$ )
- T-components ( $P_{xy}$ ,  $P_{xz}$ ...) determined at  $\pm 0.010$

Exemples:  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ,  $\text{CuGeO}_3$ ,  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ ,  $\text{BaCo}_2(\text{AsO}_4)_2$ , ...

# High-field configuration



CEA/12-T magnet on IN22 (pol. neutrons)

- Polarized neutron at 12 T  
possible but difficult  
(require optimized flippers)

- The 12-T and 15-T cryomagnets  
can be easily used on IN22

**@ H=15 T:**  
**Vertical force: < 110 kg**  
**Horizontal force: < 30 kg**



ILL/15-T magnet on IN22 (unpol. Neutrons)

# Conclusion

- Heusler-based solution was the best in the IN22 particular case:
  - Only vertical focusing (30-mm wide SM guide)
  - Incident neutron energies in the range  $5\text{meV} < E_i < 90 \text{ meV}$
  - Weak  $2k_i, 3k_i, \dots$  contaminations for  $E_i > 25 \text{ meV}$  (guide cut-off)
  - Easy high-magnetic-field, SNP or NRSE measurements
  - Stability of the polarization (ex: inelastic SNP)
- This conclusion may not be true in general:
  - TAS on a beam tube (ex: IN20@ILL, BT7@NIST,...)
  - Large-size double focusing incident beam
  - Incident neutron energies  $E_i \gg 100 \text{ meV}$
  - P and T tunable (up to some extent!)
  - Variable resolution required (PG/Si, Cu,...)
  - Elimination of  $2k_i$  (ex: Si111+ $^3\text{He}$ -NSF)
  - Possibility to install the  $^3\text{He}$ -NSF inside the monochromator shielding
  - $P_{^3\text{He}} \sim 70\text{-}75\%$  over several days
  - ...

# Conclusion

- Heusler-based solution was the best for IN22  
(only vertical focusing,  $E_i < 90$  meV, high magnetic fields, SNP and NRSE options)

	PROS	CONS
HEUSLER	<ul style="list-style-type: none"><li>- Reliability</li><li>- Stability (<math>P(t)</math>, <math>T(t)</math> constant)</li><li>- Compactness</li><li>- Simplicity of use</li><li>- Flux/polarisation ratio</li><li>- Low background</li><li>- Weak sensitivity to parasitic H</li></ul>	<ul style="list-style-type: none"><li>- <math>2k_i, 3 k_i, \dots</math> unpolarized</li><li>- Variable double focusing difficult (due to vertical magnetic forces)</li><li>- Difficult for monoch height <math>&gt; 15</math> cm (magnetic circuit too big)</li><li>- Fixed <math>d_M \approx 3.45</math> Å; Resolution</li></ul>
3He-NSF	<ul style="list-style-type: none"><li>- Optimized double focusing</li><li>- Large size monochromator</li><li>- Tunable flux/polarisation ratio</li><li>- With Si111: no <math>2k_i</math></li><li>- Variable <math>d_M</math> and resolution (Cu111: <math>\approx 2.08</math> Å, PG002, Si111 <math>\approx 3.4</math> Å)</li></ul>	<ul style="list-style-type: none"><li>- Reliability/brittleness (?)</li><li>- Complexity</li><li>- Compactness less optimized</li><li>- <math>T(k_i)</math> and <math>P(k_i)</math></li><li>- <math>^3\text{He}</math> polarization decay (<math>P(t), T(t)</math>)</li><li>- Sensitivity to parasitic fields</li><li>- Background produced by the cell</li></ul>

# Longitudinal Polarization Analysis (LPA) (Cross sections)

$$\sigma_x^{++} \propto N$$

$$\sigma_x^{--} \propto N$$

$$\sigma_x^{+-} \propto M_{yy} + M_{zz} - M_{ch}$$

$$\sigma_x^{-+} \propto M_{yy} + M_{zz} + M_{ch}$$

$$\sigma_y^{++} \propto N + M_{yy} + R_y$$

$$\sigma_y^{--} \propto N + M_{yy} - R_y$$

$$\sigma_y^{+-} \propto M_{zz}$$

$$\sigma_y^{-+} \propto M_{zz}$$

$$\sigma_z^{++} \propto N + M_{zz} + R_z$$

$$\sigma_z^{--} \propto N + M_{zz} - R_z$$

$$\sigma_z^{+-} \propto M_{yy}$$

$$\sigma_z^{-+} \propto M_{yy}$$

$$\sigma_x^{0+} \propto N + M_{yy} + M_{zz} + M_{ch}$$

$$\sigma_x^{0-} \propto N + M_{yy} + M_{zz} - M_{ch}$$

$$\sigma_y^{0+} \propto N + M_{yy} + M_{zz} + R_y$$

$$\sigma_y^{0-} \propto N + M_{yy} + M_{zz} - R_y$$

$$\sigma_z^{0+} \propto N + M_{yy} + M_{zz} + R_z$$

$$\sigma_z^{0-} \propto N + M_{yy} + M_{zz} - R_z$$

$$\sigma_x^{+0} \propto N + M_{yy} + M_{zz} - M_{ch}$$

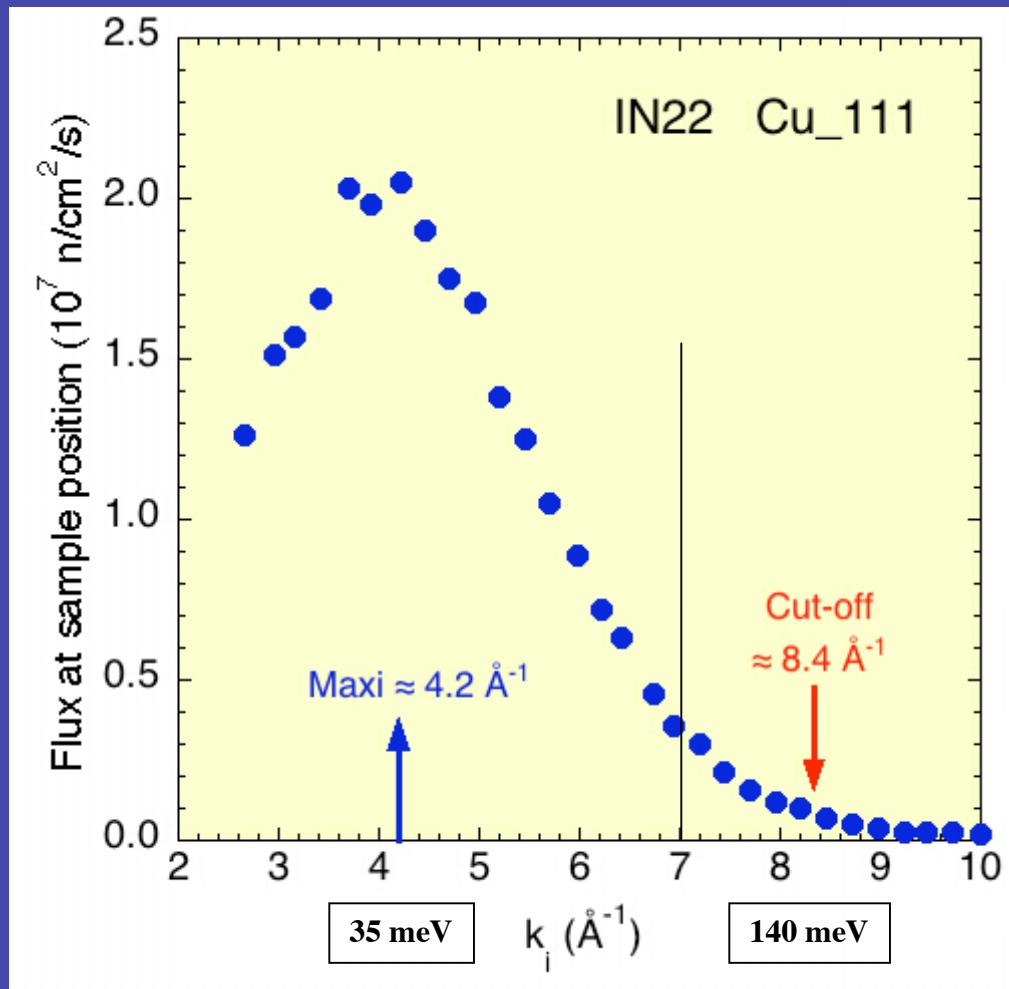
$$\sigma_x^{-0} \propto N + M_{yy} + M_{zz} + M_{ch}$$

$$\sigma_y^{+0} \propto N + M_{yy} + M_{zz} + R_y$$

$$\sigma_y^{-0} \propto N + M_{yy} + M_{zz} - R_y$$

Definition:  $\mathbf{x} \parallel \mathbf{Q}$ ,  $\mathbf{y}$  and  $\mathbf{z} \perp \mathbf{Q}$

# Flux( $k_i$ ) on IN22: Cu111 monochromator



$k_i \approx 2 \text{ \AA}^{-1} \longrightarrow \approx 7 \text{ \AA}^{-1}$

$E_i \approx 8 \text{ meV} \longrightarrow \approx 100 \text{ meV}$

Energy transfers  $< 70 \text{ meV}$

## $^3\text{He}$ -Spin-Filter option on IN22

### Filter quality :

$$P = \tanh(O.P_{^3\text{He}})$$

$$T = \exp(-O).\cosh(O.P_{^3\text{He}})$$

$$O = 0.0733 \text{ p(bar)} l(\text{cm}) \lambda(\text{\AA})$$

Depending on  $\lambda$ , the pressure inside the cell (p) can be adjusted to reach the expected neutron polarisation (P).

**Increasing the polarisation => decreasing the transmission.**

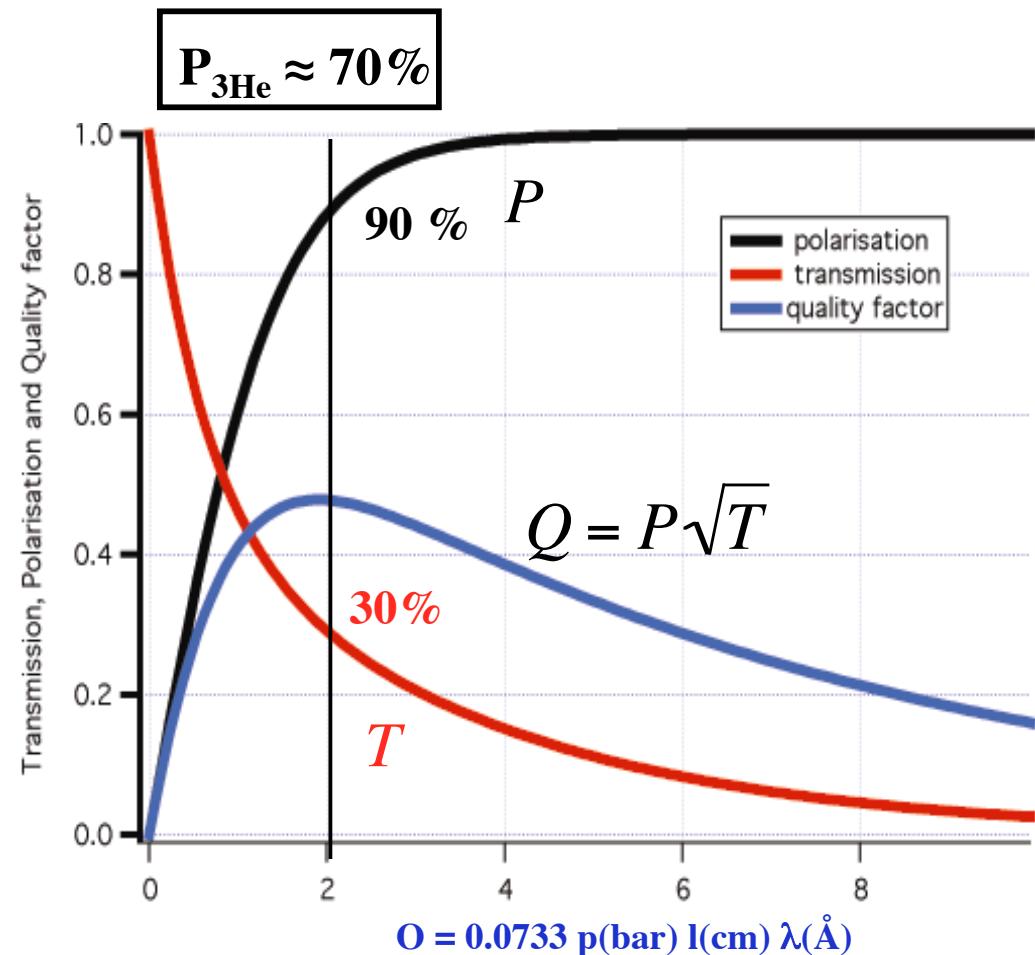
### Optimum:

$$p.l.\lambda \approx 25 \text{ (bar, cm, \AA)}$$

$$\lambda \approx 1 \text{ \AA}, l \approx 10 \text{ cm} \rightarrow p \approx 2.5 \text{ bar}$$

$$\lambda \approx 2.4 \text{ \AA}, l \approx 10 \text{ cm} \rightarrow p \approx 1 \text{ bar}$$

$$\lambda \approx 4 \text{ \AA}, l \approx 10 \text{ cm} \rightarrow p \approx 0.6 \text{ bar}$$

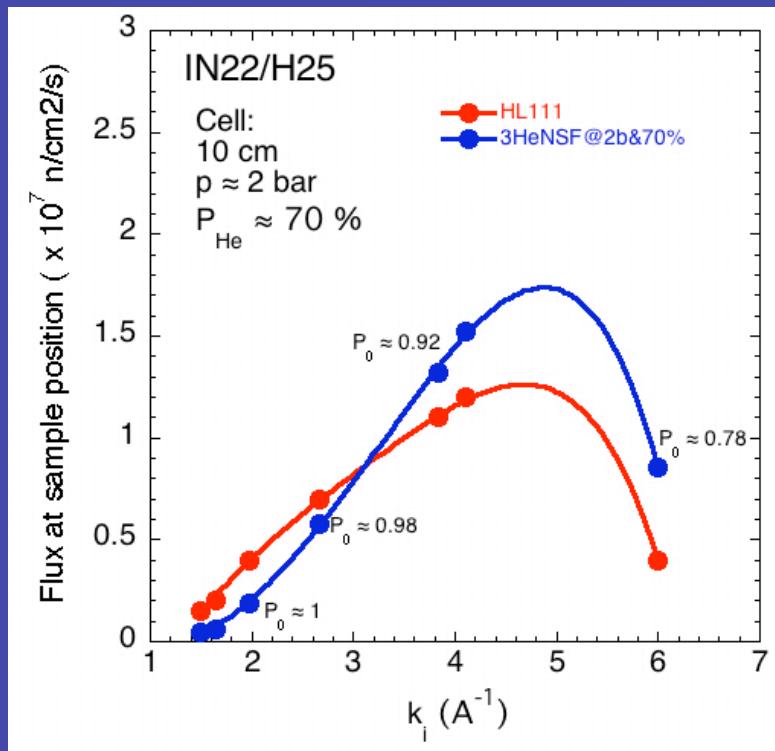


$^3\text{He-NSF}$ :  $P \approx 90\%, T \approx 30\%$

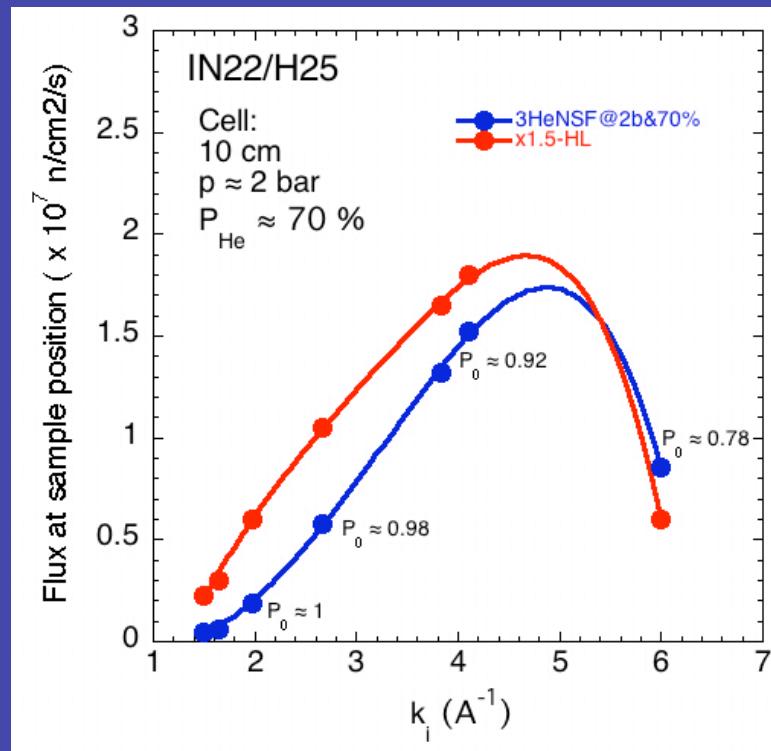
Heusler:  $P \approx 90\%, T \approx 20\%$

## Flux at sample: HL111 versus PG002&NSF

(pressure in the cell fixed at 2 bar)



With "standard" Heusler  $X^{tals}$



With "improved" Heusler  $X^{tals}$   
(reflectivity x1.5)

The choice for the particular case of IN22 (no horizontal focusing!):  
Heusler-based polarizer with "improved" Heusler crystals